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FILE 'HOME' ENTERED AT 10:09:32 ON 15 APR 2003

=> reg

REG IS NOT A RECOGNIZED COMMAND

The previous command name entered was not recognized by the system. For a list of commands available to you in the current file, enter "HELP COMMANDS" at an arrow prompt (=>).

=> fil reg

COST IN U.S. DOLLARS SINCE FILE TOTAL

ENTRY SESSION

FULL ESTIMATED COST 0.21 0.21

FILE 'REGISTRY' ENTERED AT 10:09:38 ON 15 APR 2003 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 14 APR 2003 HIGHEST RN 502958-40-9 DICTIONARY FILE UPDATES: 14 APR 2003 HIGHEST RN 502958-40-9

TSCA INFORMATION NOW CURRENT THROUGH MAY 20, 2002

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details: http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

=>
Uploading integrin antagonist.str

L1 STRUCTURE UPLOADED

=> d

L1 HAS NO ANSWERS

L1 STR

Structure attributes must be viewed using STN Express query preparation.

=> S
ENTER LOGIC EXPRESSION, QUERY NAME, OR (END):11
SAMPLE SEARCH INITIATED 10:10:03 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 13 TO ITERATE

100.0% PROCESSED 13 ITERATIONS 0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 44 TO 47

PROJECTED ITERATIONS: 44 TO 476
PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

=> s l1 full

FULL SEARCH INITIATED 10:10:10 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 266 TO ITERATE

100.0% PROCESSED 266 ITERATIONS 6 ANSWERS SEARCH TIME: 00.00.01

L3 6 SEA SSS FUL L1

=> d tot

L3 ANSWER 1 OF 6 REGISTRY COPYRIGHT 2003 ACS

RN 290826-70-9 REGISTRY

CN .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(3-bromo-5-chloro-2-hydroxyphenyl)-, (3S)-, mono(trifluoroacetate) (salt) (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C22 H23 Br Cl N5 O7 . C2 H F3 O2

SR CA

LC STN Files: CA, CAPLUS, DRUGUPDATES, TOXCENTER, USPATFULL

CM 1

CRN 243135-72-0

CMF C22 H23 Br Cl N5 O7

Absolute stereochemistry.

CM 2

CRN 76-05-1 CMF C2 H F3 O2

4 REFERENCES IN FILE CA (1962 TO DATE)

4 REFERENCES IN FILE CAPLUS (1962 TO DATE)

ANSWER 2 OF 6 REGISTRY COPYRIGHT 2003 ACS L3

RN290826-65-2 REGISTRY

.beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-CNpyrimidinyl) amino] benzoyl] glycyl-3-(3-bromo-5-chloro-2-hydroxyphenyl)-, (3R) -, compd. with trifluoromethanol (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

Methanol, trifluoro-, compd. with (3R)-N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(3-bromo-5-chloro-2hydroxyphenyl) - .beta. -alanine (9CI)

FS STEREOSEARCH

MF C22 H23 Br Cl N5 O7 . \times C H F3 O

SR CA

LC STN Files: CA, CAPLUS, DRUGUPDATES, USPATFULL

CM 1

CRN 280105-17-1

CMF C22 H23 Br Cl N5 O7

Absolute stereochemistry.

$$\begin{array}{c|c} & & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ &$$

CM 2

CRN 1493-11-4 CMF C H F3 O

2 REFERENCES IN FILE CA (1962 TO DATE)
2 REFERENCES IN FILE CAPLUS (1962 TO DATE)

L3 ANSWER 3 OF 6 REGISTRY COPYRIGHT 2003 ACS

RN 280105-17-1 REGISTRY

CN .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(3-bromo-5-chloro-2-hydroxyphenyl)-, (3R)- (9CI) (CA INDEX NAME)

OTHER NAMES:

CN SD 7784

FS STEREOSEARCH

MF C22 H23 Br Cl N5 O7

CI COM

SR CA

LC STN Files: CA, CAPLUS, DRUGUPDATES, TOXCENTER

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- 6 REFERENCES IN FILE CA (1962 TO DATE)
- 1 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
- 6 REFERENCES IN FILE CAPLUS (1962 TO DATE)
- L3 ANSWER 4 OF 6 REGISTRY COPYRIGHT 2003 ACS
- RN 243135-82-2 REGISTRY
- CN .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(3-bromo-5-chloro-2-hydroxyphenyl)-, monohydrochloride, (3S)- (9CI) (CA INDEX NAME)
- FS STEREOSEARCH
- MF C22 H23 Br Cl N5 O7 . Cl H
- SR CA
- LC STN Files: CA, CAPLUS, DRUGUPDATES, TOXCENTER, USPATFULL
- CRN (243135-72-0)

Absolute stereochemistry.

• HCl

- 2 REFERENCES IN FILE CA (1962 TO DATE)
- 2 REFERENCES IN FILE CAPLUS (1962 TO DATE)
- L3 ANSWER 5 OF 6 REGISTRY COPYRIGHT 2003 ACS
- RN 243135-73-1 REGISTRY
- CN .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(3-bromo-5-chloro-2-hydroxyphenyl)-, (3S)-, trifluoroacetate (10:17) (salt) (9CI) (CA INDEX NAME)
- FS STEREOSEARCH
- MF C22 H23 Br Cl N5 O7 . 17/10 C2 H F3 O2
- SR CA
- LC STN Files: CA, CAPLUS, DRUGUPDATES, TOXCENTER, USPATFULL

CM 1

CRN 243135-72-0

CMF C22 H23 Br Cl N5 O7

Absolute stereochemistry.

$$\begin{array}{c|c} H & H & O & H & S \\ \hline N & N & N & O & OH \\ \hline OH & OH & CO_2H & CO_2H \\ \end{array}$$

CM 2

CRN 76-05-1 CMF C2 H F3 O2

3 REFERENCES IN FILE CA (1962 TO DATE)

3 REFERENCES IN FILE CAPLUS (1962 TO DATE)

L3 ANSWER 6 OF 6 REGISTRY COPYRIGHT 2003 ACS

RN 243135-72-0 REGISTRY

CN .beta.-Alanine, N-[3-hydroxy-5-[(1,4,5,6-tetrahydro-5-hydroxy-2-pyrimidinyl)amino]benzoyl]glycyl-3-(3-bromo-5-chloro-2-hydroxyphenyl)-, (3S)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C22 H23 Br Cl N5 O7

CI COM

SR CA

LC STN Files: CA, CAPLUS, DRUGNL, DRUGUPDATES, TOXCENTER, USPATFULL

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT